Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2025 – 06:22 PM JST

PDB ID	:	8Z0H
Title	:	Crystal structure of 9-mer peptide from ALV-J in complex with BF2*0201
Authors	:	Jia, Y.S.; Ma, M.L.; Li, Y.L.; Liao, M.; Dai, M.M.
Deposited on	:	2024-04-09
Resolution	:	1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

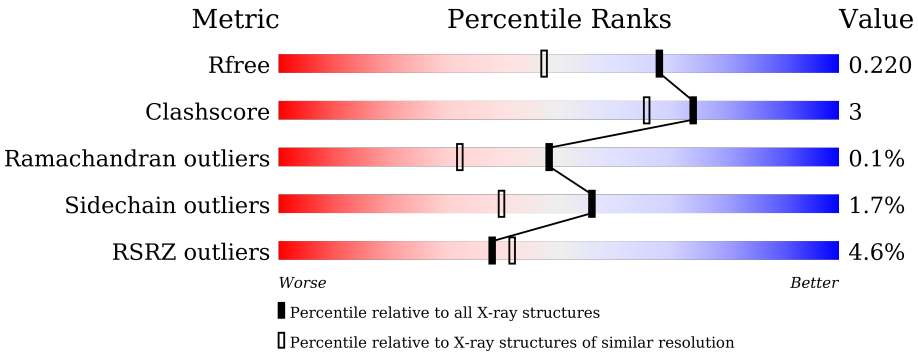
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7106 (1.74-1.70)
Clashscore	180529	7746 (1.74-1.70)
Ramachandran outliers	177936	7654 (1.74-1.70)
Sidechain outliers	177891	7654 (1.74-1.70)
RSRZ outliers	164620	7104 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	273	5% 95% 5%
1	D	273	4% 95% 5%
1	G	273	4% 95% 5%
1	J	273	5% 93% 6%
2	B	97	86% 14%
2	E	97	% 89% 11%

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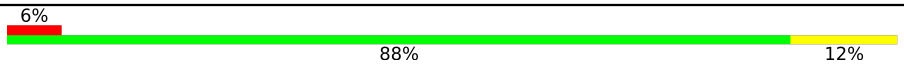
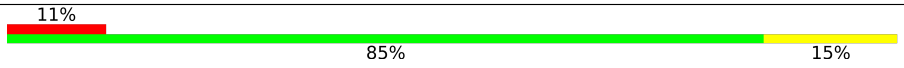
Mol	Chain	Length	Quality of chain
2	H	97	
2	K	97	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13619 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MHC class I alpha chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2202	1390	389	414	9			
1	D	273	Total	C	N	O	S	0	0	0
			2202	1390	389	414	9			
1	G	273	Total	C	N	O	S	0	0	0
			2202	1390	389	414	9			
1	J	273	Total	C	N	O	S	0	0	0
			2202	1390	389	414	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O46789
D	0	MET	-	initiating methionine	UNP O46789
G	0	MET	-	initiating methionine	UNP O46789
J	0	MET	-	initiating methionine	UNP O46789

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			771	495	125	146	5			
2	E	97	Total	C	N	O	S	0	0	0
			771	495	125	146	5			
2	H	97	Total	C	N	O	S	0	0	0
			771	495	125	146	5			
2	K	97	Total	C	N	O	S	0	0	0
			770	495	125	145	5			

- Molecule 3 is a protein called Gag protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	I	9	Total C N O 72 45 13 14	0	0	0
3	C	9	Total C N O 72 45 13 14	0	0	0
3	F	9	Total C N O 72 45 13 14	0	0	0
3	L	9	Total C N O 72 45 13 14	0	0	0

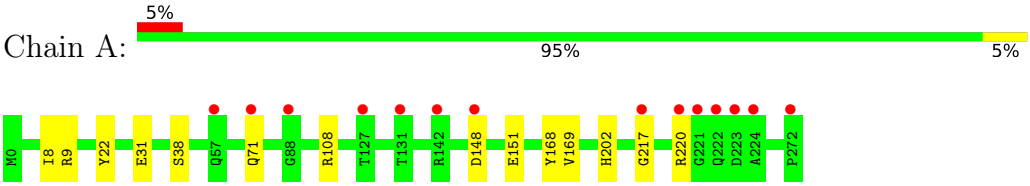
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	233	Total O 233 233	0	0
4	B	119	Total O 119 119	0	0
4	D	252	Total O 252 252	0	0
4	E	125	Total O 125 125	0	0
4	G	269	Total O 269 269	0	0
4	H	95	Total O 95 95	0	0
4	J	230	Total O 230 230	0	0
4	K	66	Total O 66 66	0	0
4	I	16	Total O 16 16	0	0
4	C	7	Total O 7 7	0	0
4	F	10	Total O 10 10	0	0
4	L	18	Total O 18 18	0	0

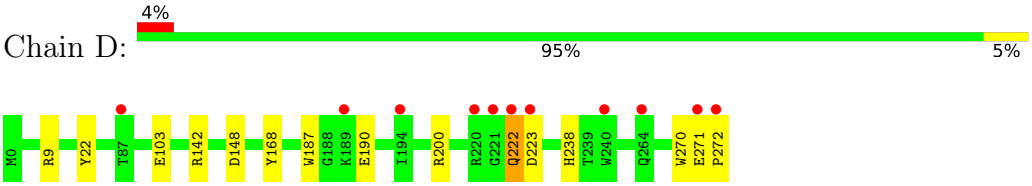
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

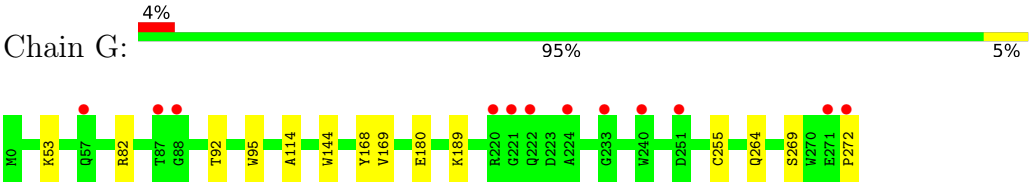
• Molecule 1: MHC class I alpha chain 2



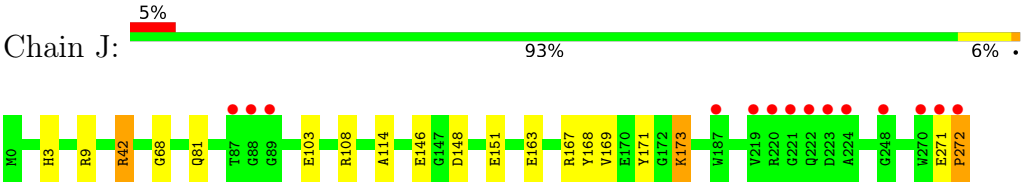
• Molecule 1: MHC class I alpha chain 2



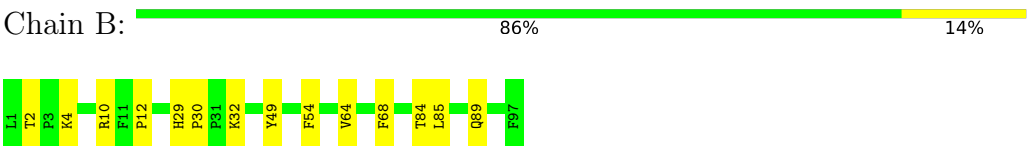
• Molecule 1: MHC class I alpha chain 2



• Molecule 1: MHC class I alpha chain 2

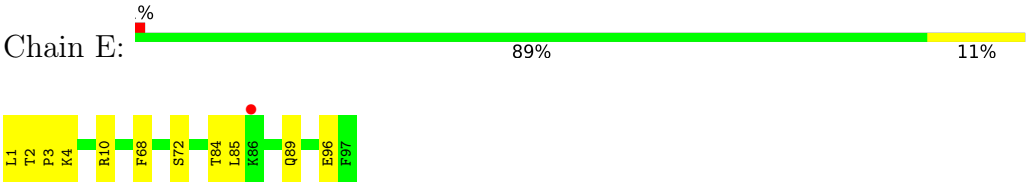


• Molecule 2: Beta-2-microglobulin



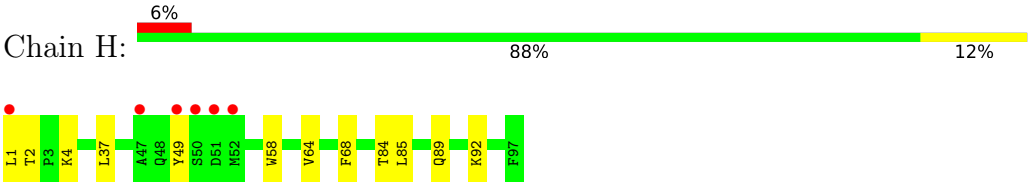
• Molecule 2: Beta-2-microglobulin

Chain E:



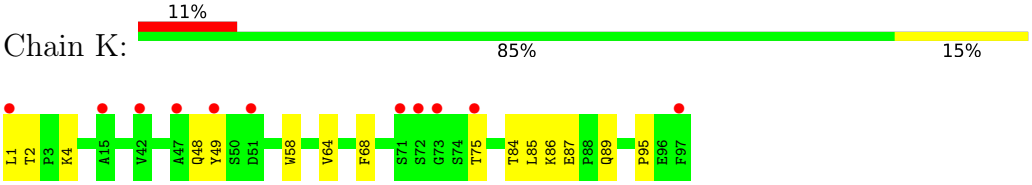
• Molecule 2: Beta-2-microglobulin

Chain H:



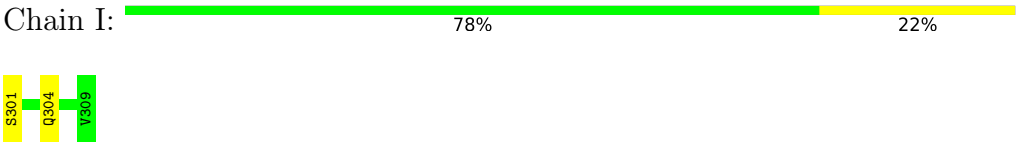
• Molecule 2: Beta-2-microglobulin

Chain K:



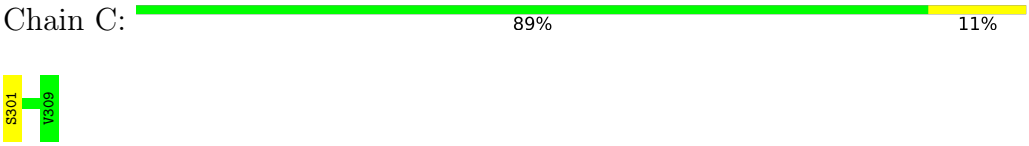
• Molecule 3: Gag protein

Chain I:



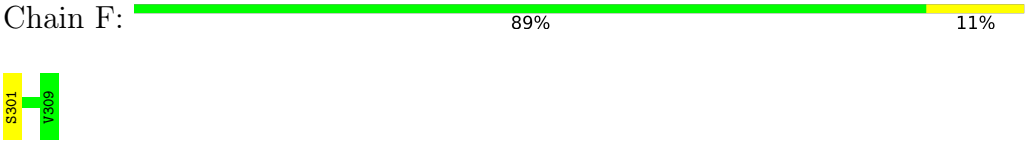
• Molecule 3: Gag protein

Chain C:



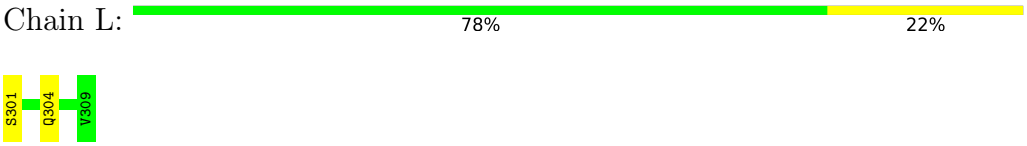
• Molecule 3: Gag protein

Chain F:



• Molecule 3: Gag protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.61Å 115.58Å 94.11Å 90.00° 111.16° 90.00°	Depositor
Resolution (Å)	87.76 – 1.72 87.76 – 1.72	Depositor EDS
% Data completeness (in resolution range)	98.7 (87.76-1.72) 98.7 (87.76-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.95 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.182 , 0.212 0.192 , 0.220	Depositor DCC
R_{free} test set	9009 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13619	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.51	0/2267	0.80	0/3081
1	D	0.53	1/2267 (0.0%)	0.79	0/3081
1	G	0.49	0/2267	0.79	0/3081
1	J	0.52	1/2267 (0.0%)	0.79	2/3081 (0.1%)
2	B	0.51	0/796	0.81	1/1081 (0.1%)
2	E	0.54	0/796	0.84	1/1081 (0.1%)
2	H	0.47	0/796	0.79	0/1081
2	K	0.48	0/795	0.81	2/1081 (0.2%)
3	C	0.56	0/72	0.66	0/94
3	F	0.76	0/72	0.77	0/94
3	I	0.62	0/72	0.74	0/94
3	L	0.98	0/72	0.84	0/94
All	All	0.52	2/12539 (0.0%)	0.80	6/17024 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	J	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	103	GLU	CD-OE2	-6.44	1.18	1.25
1	J	103	GLU	CD-OE1	5.12	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	95	PRO	C-N-CA	-7.48	103.00	121.70
2	B	10	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	J	171	TYR	CB-CG-CD2	-5.26	117.84	121.00
2	K	95	PRO	N-CA-C	-5.18	98.62	112.10
1	J	9	ARG	CB-CA-C	-5.15	100.10	110.40
2	E	10	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	220	ARG	Sidechain
1	J	108	ARG	Sidechain
1	J	42	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2202	0	2071	9	0
1	D	2202	0	2071	9	1
1	G	2202	0	2071	12	0
1	J	2202	0	2071	11	1
2	B	771	0	733	8	0
2	E	771	0	733	11	0
2	H	771	0	733	10	0
2	K	770	0	733	13	0
3	C	72	0	70	1	0
3	F	72	0	70	1	0
3	I	72	0	70	1	0
3	L	72	0	70	2	0
4	A	233	0	0	4	0
4	B	119	0	0	1	0
4	C	7	0	0	0	0
4	D	252	0	0	1	0
4	E	125	0	0	2	0
4	F	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	269	0	0	8	0
4	H	95	0	0	3	0
4	I	16	0	0	0	0
4	J	230	0	0	3	0
4	K	66	0	0	2	0
4	L	18	0	0	0	0
All	All	13619	0	11496	72	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:72:SER:OG	1:J:272:PRO:O	1.94	0.85
1:G:180:GLU:HG2	4:G:325:HOH:O	1.76	0.84
2:H:1:LEU:HA	4:H:179:HOH:O	1.85	0.75
1:A:169:VAL:HG13	4:A:473:HOH:O	1.88	0.73
1:G:168:TYR:HH	3:I:301:SER:N	1.85	0.73
1:G:169:VAL:HG13	4:G:455:HOH:O	1.92	0.70
1:J:168:TYR:HH	3:L:301:SER:N	1.88	0.70
1:J:163:GLU:OE2	1:J:167:ARG:NH2	2.25	0.69
1:G:255:CYS:SG	4:G:524:HOH:O	2.51	0.68
1:D:190:GLU:HG3	2:K:75:THR:HG21	1.76	0.68
1:A:168:TYR:HH	3:C:301:SER:N	1.92	0.67
1:D:168:TYR:HH	3:F:301:SER:N	1.95	0.65
2:E:72:SER:CB	1:J:272:PRO:O	2.48	0.60
1:D:270:TRP:O	1:D:272:PRO:HD3	2.02	0.58
1:A:31:GLU:HG3	4:A:462:HOH:O	2.03	0.58
2:K:89:GLN:NE2	4:K:101:HOH:O	2.32	0.58
2:K:1:LEU:HA	4:K:152:HOH:O	2.04	0.57
1:G:180:GLU:CG	4:G:325:HOH:O	2.41	0.57
1:J:81:GLN:CD	4:J:301:HOH:O	2.43	0.56
1:D:190:GLU:CG	2:K:75:THR:HG21	2.37	0.54
2:H:92:LYS:HD3	4:H:187:HOH:O	2.07	0.54
2:H:1:LEU:N	2:H:1:LEU:HD12	2.23	0.54
1:A:151:GLU:HG2	4:A:313:HOH:O	2.08	0.54
2:H:85:LEU:HD13	2:H:89:GLN:HG3	1.91	0.52
2:E:1:LEU:HD12	2:E:1:LEU:N	2.25	0.52
2:B:85:LEU:HD13	2:B:89:GLN:HG3	1.91	0.52
1:G:92:THR:HG23	4:G:366:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:LEU:HD13	2:E:89:GLN:HG3	1.92	0.51
1:G:95:TRP:HH2	1:G:144:TRP:HH2	1.59	0.51
1:G:189:LYS:HE3	4:G:529:HOH:O	2.11	0.51
2:H:49:TYR:CD2	2:H:64:VAL:HG22	2.47	0.49
1:A:217:GLY:HA2	4:A:506:HOH:O	2.13	0.49
1:D:142:ARG:NH1	4:D:308:HOH:O	2.45	0.49
1:G:255:CYS:HB3	4:G:524:HOH:O	2.13	0.48
2:B:49:TYR:CD2	2:B:64:VAL:HG22	2.49	0.48
2:E:1:LEU:HA	4:E:200:HOH:O	2.13	0.48
2:K:49:TYR:CD2	2:K:64:VAL:HG22	2.49	0.48
1:G:82:ARG:O	4:G:301:HOH:O	2.20	0.48
1:J:146:GLU:HG3	4:J:445:HOH:O	2.13	0.47
2:H:1:LEU:N	2:H:1:LEU:CD1	2.78	0.47
2:K:1:LEU:HD12	2:K:1:LEU:N	2.30	0.47
1:D:200:ARG:HG2	1:D:238:HIS:CE1	2.51	0.46
1:J:173:LYS:HE2	4:J:303:HOH:O	2.15	0.46
1:A:9:ARG:HD2	1:A:22:TYR:OH	2.17	0.45
2:B:2:THR:HG22	2:B:84:THR:HB	1.98	0.45
2:K:2:THR:HG22	2:K:84:THR:HB	1.98	0.45
2:E:72:SER:HB2	1:J:272:PRO:O	2.14	0.45
2:H:1:LEU:CD1	2:H:1:LEU:H3	2.30	0.45
2:H:2:THR:HG22	2:H:84:THR:HB	1.98	0.45
2:K:4:LYS:N	2:K:4:LYS:HD2	2.32	0.45
1:J:68:GLY:HA3	3:L:304:GLN:HE22	1.83	0.44
2:H:1:LEU:CA	4:H:179:HOH:O	2.55	0.44
2:E:1:LEU:N	2:E:1:LEU:CD1	2.80	0.43
2:K:1:LEU:N	2:K:1:LEU:CD1	2.80	0.43
2:K:86:LYS:HB2	2:K:87:GLU:OE1	2.18	0.43
2:E:1:LEU:CD1	4:E:213:HOH:O	2.67	0.43
1:A:8:ILE:HB	2:B:54:PHE:CZ	2.54	0.43
1:J:114:ALA:HB2	2:K:58:TRP:CE2	2.53	0.43
2:K:85:LEU:HD13	2:K:89:GLN:HG3	2.00	0.43
1:D:9:ARG:HD2	1:D:22:TYR:OH	2.19	0.42
1:G:114:ALA:HB2	2:H:58:TRP:CE2	2.54	0.42
2:B:32:LYS:HD2	4:B:117:HOH:O	2.20	0.42
1:A:22:TYR:HB3	1:A:38:SER:HB3	2.01	0.42
2:B:4:LYS:N	2:B:4:LYS:HD2	2.34	0.42
1:J:3:HIS:CG	1:J:169:VAL:HG11	2.55	0.42
1:D:190:GLU:HG3	2:K:75:THR:CG2	2.46	0.41
2:E:1:LEU:CD1	2:E:1:LEU:H3	2.34	0.41
2:E:2:THR:HG22	2:E:84:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:HIS:CD2	2:B:12:PRO:HG3	2.56	0.41
2:B:29:HIS:CD2	2:B:30:PRO:HA	2.55	0.41
1:D:187:TRP:CE2	2:E:96:GLU:HA	2.57	0.40
1:G:269:SER:HB2	1:G:272:PRO:HA	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:GLN:OE1	1:J:151:GLU:OE1[1_655]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	271/273 (99%)	269 (99%)	2 (1%)	0	100 100
1	D	271/273 (99%)	265 (98%)	4 (2%)	2 (1%)	19 7
1	G	271/273 (99%)	268 (99%)	3 (1%)	0	100 100
1	J	271/273 (99%)	266 (98%)	5 (2%)	0	100 100
2	B	95/97 (98%)	95 (100%)	0	0	100 100
2	E	95/97 (98%)	94 (99%)	1 (1%)	0	100 100
2	H	95/97 (98%)	95 (100%)	0	0	100 100
2	K	95/97 (98%)	94 (99%)	1 (1%)	0	100 100
3	C	7/9 (78%)	7 (100%)	0	0	100 100
3	F	7/9 (78%)	7 (100%)	0	0	100 100
3	I	7/9 (78%)	7 (100%)	0	0	100 100
3	L	7/9 (78%)	7 (100%)	0	0	100 100
All	All	1492/1516 (98%)	1474 (99%)	16 (1%)	2 (0%)	48 32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	271	GLU
1	D	223	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	223/223 (100%)	221 (99%)	2 (1%)	75 67
1	D	223/223 (100%)	221 (99%)	2 (1%)	75 67
1	G	223/223 (100%)	221 (99%)	2 (1%)	75 67
1	J	223/223 (100%)	218 (98%)	5 (2%)	47 29
2	B	85/85 (100%)	84 (99%)	1 (1%)	67 55
2	E	85/85 (100%)	82 (96%)	3 (4%)	31 13
2	H	85/85 (100%)	82 (96%)	3 (4%)	31 13
2	K	85/85 (100%)	83 (98%)	2 (2%)	44 25
3	C	7/7 (100%)	7 (100%)	0	100 100
3	F	7/7 (100%)	7 (100%)	0	100 100
3	I	7/7 (100%)	6 (86%)	1 (14%)	2 0
3	L	7/7 (100%)	7 (100%)	0	100 100
All	All	1260/1260 (100%)	1239 (98%)	21 (2%)	56 40

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	148	ASP
2	B	68	PHE
1	D	148	ASP
1	D	222	GLN
2	E	3	PRO
2	E	4	LYS

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Mol	Chain	Res	Type
2	E	68	PHE
1	G	53	LYS
1	G	264	GLN
2	H	4	LYS
2	H	37	LEU
2	H	68	PHE
1	J	42	ARG
1	J	148	ASP
1	J	173	LYS
1	J	271	GLU
1	J	272	PRO
2	K	48	GLN
2	K	68	PHE
3	I	304	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	222	GLN
2	E	61	GLN
2	E	89	GLN
1	G	225	HIS
1	J	222	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	273/273 (100%)	0.26	14 (5%) 34 38	10, 19, 38, 70	0
1	D	273/273 (100%)	0.05	11 (4%) 43 47	10, 17, 38, 87	0
1	G	273/273 (100%)	0.09	12 (4%) 39 43	11, 18, 36, 85	0
1	J	273/273 (100%)	0.12	14 (5%) 34 38	9, 17, 42, 96	0
2	B	97/97 (100%)	-0.17	0 100 100	10, 15, 28, 43	0
2	E	97/97 (100%)	-0.16	1 (1%) 79 82	10, 15, 27, 52	0
2	H	97/97 (100%)	0.33	6 (6%) 28 30	14, 20, 40, 47	0
2	K	97/97 (100%)	0.84	11 (11%) 11 12	14, 26, 46, 57	0
3	C	9/9 (100%)	0.15	0 100 100	17, 23, 28, 33	0
3	F	9/9 (100%)	-0.17	0 100 100	12, 20, 21, 24	0
3	I	9/9 (100%)	-0.16	0 100 100	15, 16, 18, 26	0
3	L	9/9 (100%)	-0.57	0 100 100	10, 13, 15, 21	0
All	All	1516/1516 (100%)	0.14	69 (4%) 38 42	9, 18, 39, 96	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	272	PRO	10.2
1	G	272	PRO	6.9
1	D	272	PRO	6.7
1	A	272	PRO	6.2
2	H	51	ASP	4.8
1	A	221	GLY	4.5
1	D	87	THR	4.2
1	D	220	ARG	4.1
1	A	223	ASP	4.1
2	H	49	TYR	3.8
2	K	97	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
2	K	51	ASP	3.6
1	A	224	ALA	3.6
2	H	50	SER	3.4
1	J	87	THR	3.3
1	D	221	GLY	3.3
1	J	221	GLY	3.3
1	A	222	GLN	3.3
1	J	248	GLY	3.2
1	D	223	ASP	3.1
1	J	220	ARG	3.1
1	D	264	GLN	3.1
1	G	87	THR	3.1
2	K	49	TYR	3.1
1	J	271	GLU	3.1
1	J	187	TRP	3.0
1	G	224	ALA	3.0
2	K	73	GLY	2.9
2	H	52	MET	2.9
1	D	222	GLN	2.8
2	K	75	THR	2.8
1	D	240	TRP	2.8
1	G	221	GLY	2.8
2	K	42	VAL	2.8
1	A	220	ARG	2.8
1	G	251	ASP	2.8
2	H	47	ALA	2.8
2	K	72	SER	2.7
1	D	189	LYS	2.7
1	D	271	GLU	2.7
1	J	224	ALA	2.6
2	K	71	SER	2.6
1	J	88	GLY	2.6
1	J	89	GLY	2.5
2	K	1	LEU	2.4
1	J	222	GLN	2.4
1	G	240	TRP	2.4
2	E	86	LYS	2.4
1	A	57	GLN	2.4
1	G	57	GLN	2.3
1	G	271	GLU	2.3
1	G	233	GLY	2.3
2	H	1	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	127	THR	2.3
1	J	270	TRP	2.3
1	J	223	ASP	2.2
1	G	88	GLY	2.2
1	A	88	GLY	2.2
1	A	148	ASP	2.2
1	G	220	ARG	2.2
1	A	71	GLN	2.2
1	A	217	GLY	2.2
2	K	15	ALA	2.1
2	K	47	ALA	2.1
1	G	222	GLN	2.1
1	J	219	VAL	2.1
1	A	131	THR	2.0
1	A	142	ARG	2.0
1	D	194	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.